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Intended for: Report

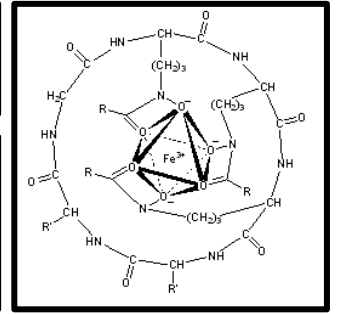
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$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Jaynesian Synthesis: Environmental Chemical Complexity

S. Elliott with Threat, Materials, Surety, Safety, COSIM, RUBISCO, LDRD

Students –A. Jayasinghe, H. Adams, A. Enders

E.T. Jaynes Meets Complex Chemistry

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$

Pragmatic but Also Formal

Laplace, Boltzmann, Gibbs, Shannon

Set Theory to Statistical Mechanics

Rank order compact schemes

Applications Thus Far

Ice giant collisions

Laboratory radiolysis

Sea surface microlayer

Boreal aquatic C

High energy Earth System pulses

Nitramines, more in progress

Some Results to Date

Giant Impact

Fischer-Tropsch chains

LMW Radiochemistry

Gem diols, trioxanes, plastics

Global Marine Roughness

Biomacromolecular monolayer

Riverine C

Light, heat, momentum, nutrients, ligs

Food Security

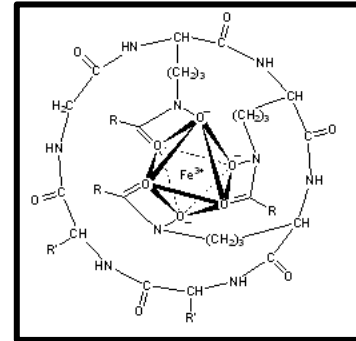
Near field sensitivity, minerals

Nitramines

Catalysis, defects, statistical EOS

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Detail: The Recipe

Common Sense Quantified

Unit hypercube

Gantt with Algorithmic Greed

Reactive probabilities

Statistical Priors with Succession

Negentropy sidesteps Cromwell

Tesler's Chemical Corollary

Experimental sweet spots

Opportunity Indices

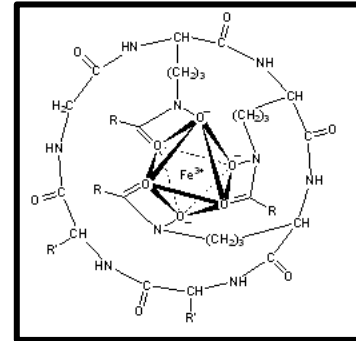
Roulette space and Shannon H

Machine learning

Unravel the mesh

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Detail: The Recipe, Formal Analogs

Normalized Sample Spaces

Unit hypercube

Königsburg, Traveling Salesman

Reactive probabilities

Entropic Availability, Evenness

Negentropy sidesteps Cromwell

Goldilocks Opportunity

Experimental sweet spots

MECE Permuted Luminance

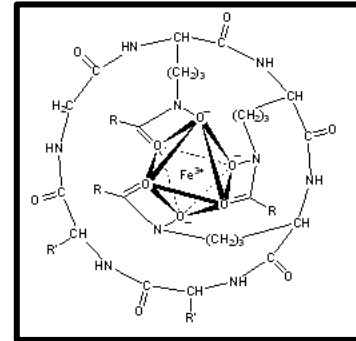
Roulette space and Shannon H

Nonbiased Cluster-Receptor Zones

Unravel the mesh

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



APPEND

Practical Issues

Let the Pantheon Write a...

Cookbook for chemistry

Conveniently Just Jaynesian

You'll love "Logic of Science"

Enviro-Chem from Ground Up

Rest is Silicon Valley

Teaming Possibilities

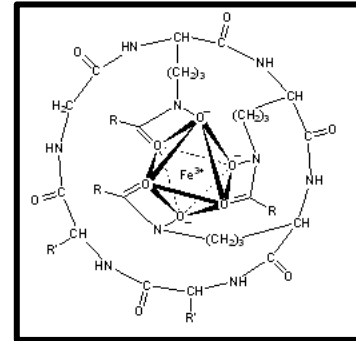
To improve inference, rigor, processes

To Quote Teller

Simplicity is just managed complexity

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Essential: Build UP from Chem KB

Foundations in Lab, Experiment

“Infer-matic” filter

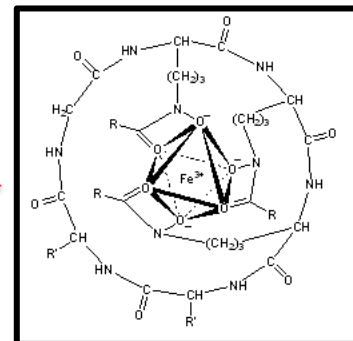
Avert curse of Cromwell

Season with fuzz, Python

Rank, test reduced models

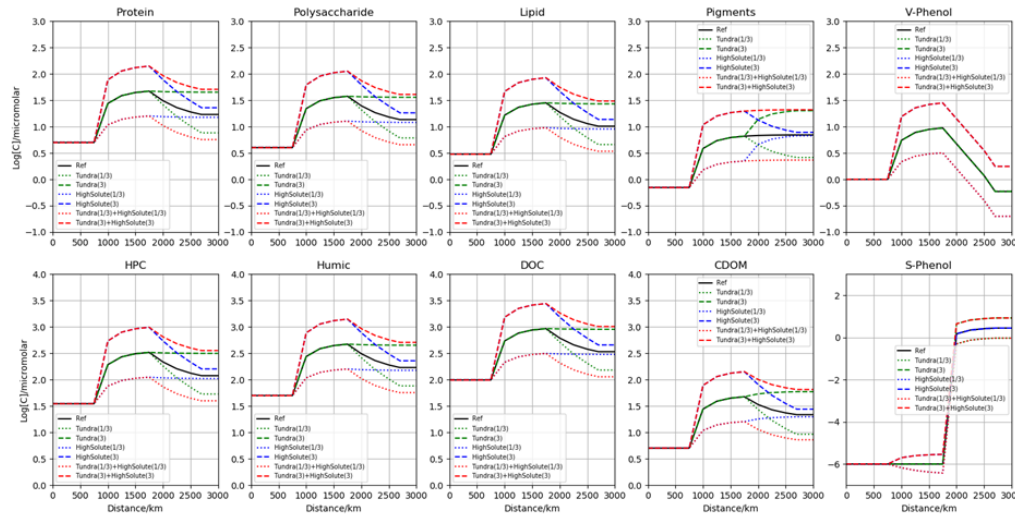
$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$

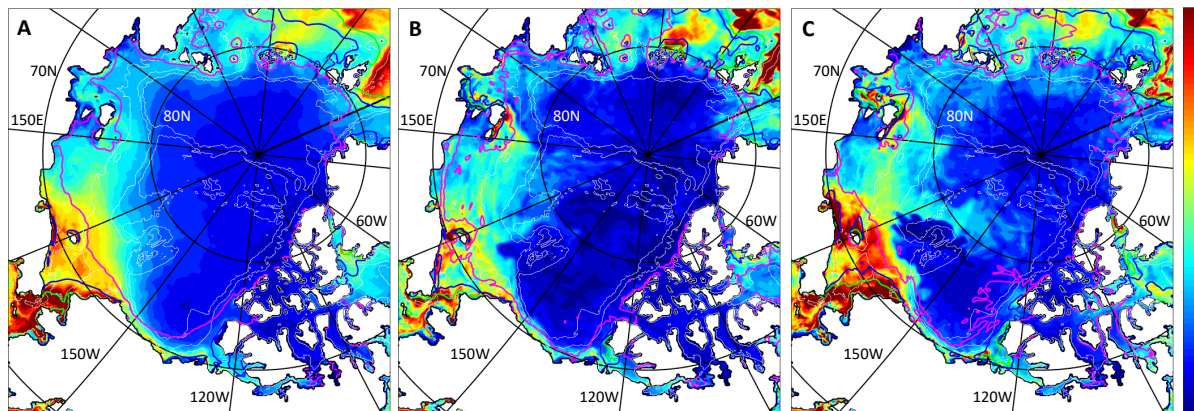
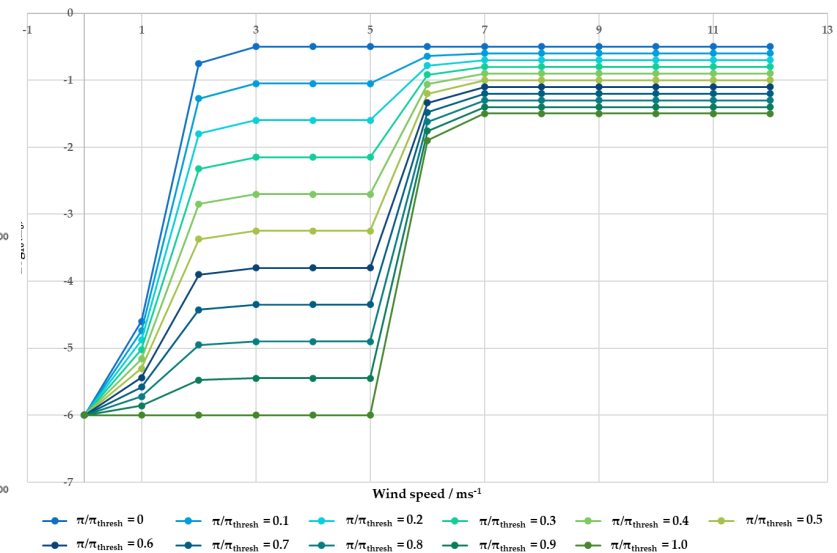


Sample Results: Boreal Organic Function

Dilution/Mixing



Plot of $\text{Log}_{10}(Z_0)$ vs Wind speed



Food Security: Set Up

Chem-Probs and Growing Season

All on unit interval

Greedy Gantt Analysis

TTAPS family, IndoPak-Levant

Urban masses, redox, Larimer

Cromwell Prior?

Upper atmosphere aerosol, ozone

Negentropy from Observation

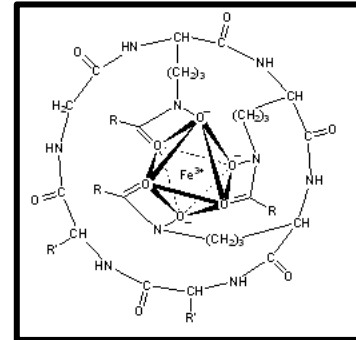
Clay, Ca, agg, steel, gypsum, volcanics

Cluster Zones

Lagrangian log-time

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



(How to Read a Greedy Gantt)

Add Probability Columns Right

Indices of reactivity

Ideally Upper Triangular Progress

Blanks of high P?

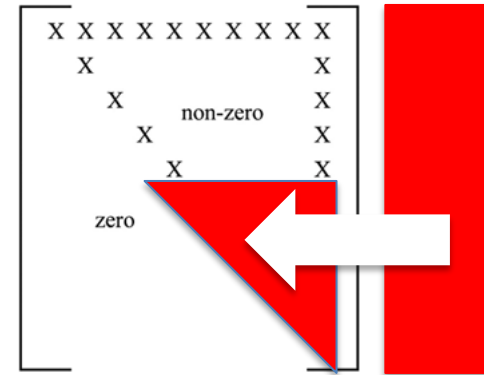
Probe via redmods

On a learned grid...

Blockage?

Lack of pedestal

Other Subtleties... Follow the Info-Entropy



Food Security: Gantt Schematic

	Hudson (etc.)	Global 1D	CARMA	CCSM	CESM	Mass	Redox	Larimer	Surface	Goldilocks
Dust	X	X	X	X	X	+				
C < IV		X	X	X	X					
Ozone				X	X					
Clay						+	-	-	+	G
Lime						+		+	+	G
Agg						+			+	G
Gypsum						+			+	G
Steel						+				G
Volcanic						+				G
Asphalt							+	+	+	G
Veg							+			G
SiO ₂						+			+	G
CaO(OH ₂)						+			+	G
Sulfate									+	G

Comments: TTAPS lineage as foil for Cromwell prior.

Central Asian urban and landscape per Lindsay, Gaffney, Sorkhabi and Davis.

Goldilocks readily observed anecdotal, Cromwell barrier above minerals.

Machine tool the regional grid, to urban to millisecond to Lagrange trajectories.

Condense, rubble, fast sticking and aerodynamics... SAIC family?

Food Security: Application

Topical Given COVID

Crops f(chem)

Gantt Analysis Says Add

Near field minerals

Machine Regrid to Lagrange

Rank reduced, SAIC

Recommended Mechanisms

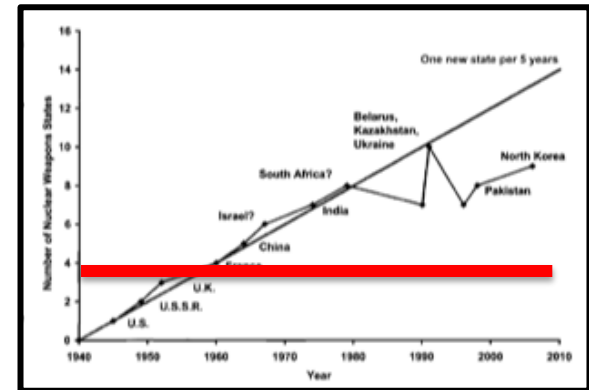
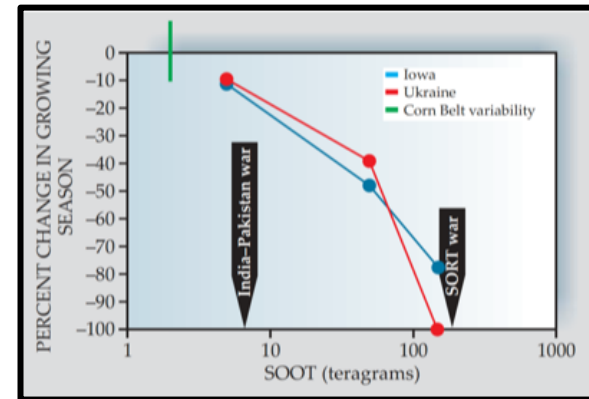
Condense, rubble, fast stick aerodyn

Sources: Central Asia Geopolitical-Chem

SIPRI, PRIO

Koppen, NDVI

Lindsay, Gaffney, Sorkhabi, Davis



Nitramine Safety

Greedy Gantt in This Case?

*Allied, Cold War, machine era
Couple chemistry to CJ-ZND*

Negentropy from Laboratories

Post-WWII, DNA, LANL/LLNL

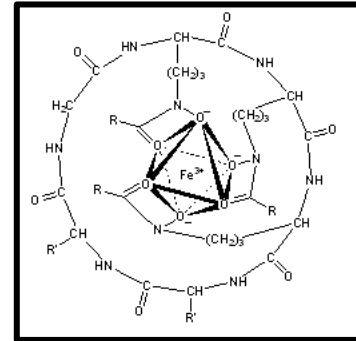
Opportunities

Relatively subtle since well-studied...

But Suggest C Chains to Ideal Statistics

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



(How to Read a GG: Redux)

Add Probability Columns Right

Indices of reactivity

Ideally Upper Triangular Progress

Blanks of high P?

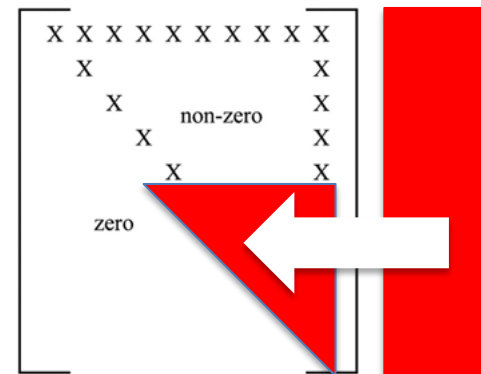
Probe via redmods

On a learned grid...

Blockage?

Lack of pedestal

Other subtleties... Follow the Info-Entropy



Safety: Gantt Schematic

	German	British	Cold War	Belt Way	Modern Lab	Comp Lab	Ergonics	ACT	Phases	Efficiency
Stoich ΔH f(state)	X	X	X X	X X	X	X X				(+) (+)
Compress f(mix)		X	X	X	X	X				(+)
Catalysis Freezeout		X X	X	X	X	X				(+)
Tune (coeffs) Vary (coeffs)		X		X	X	X				(+) (+)
C phases Binders (poly)					X		+	+	+	
Exponent form Stat mech virial					X				+	+
Defects Extra LMW ΔH					X X	--		+	+	+
Python ecosys level					X					+
Kilospecies Kiloparticles						X X				
Tailor intermol- dynamics (MD)						X				

Comments: References in JWL lineage, available on request. Parentheses implicit. Work in progress will evolve, but upper triangle blanks now BEHIND the diagonal. Suggestive of needs for lab study chained C, defect structure and... Statistical Mechanical virials and idealizations as an expedient.

HMX: Specific Chemical Issues

WWII observations

Fragment catalysis, freeze

Alternate C Oxidation States

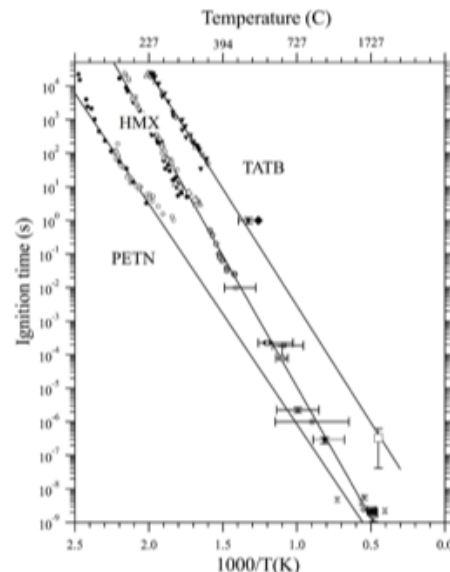
Polymeric binders

Defects as nucleii

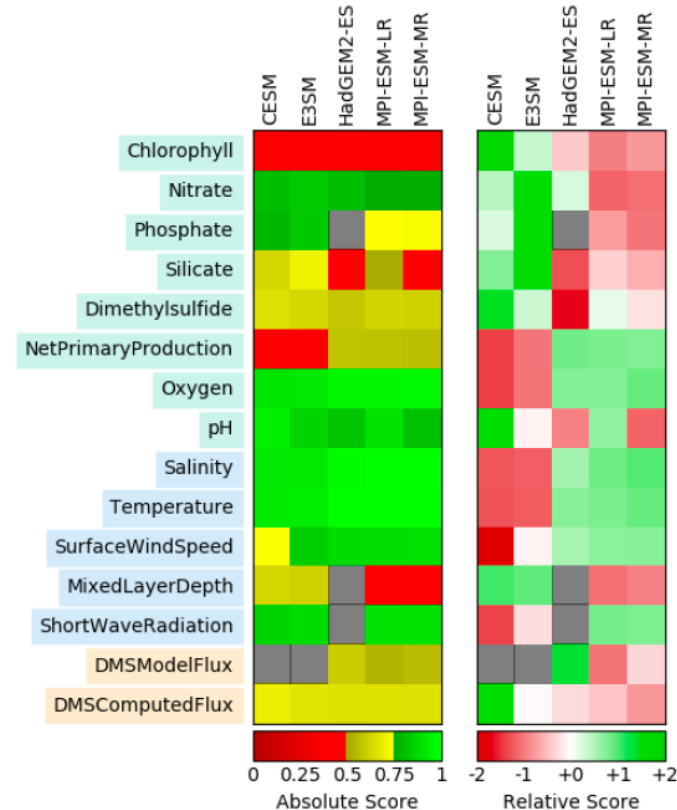
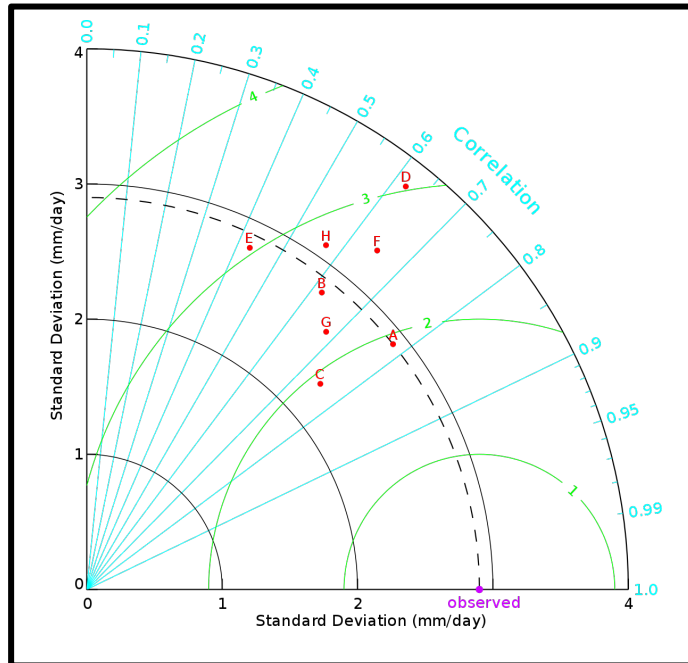
Pseudo-fluids and their statistics

Extra enthalpic channels

Higher than LMW



Complement Pearson-Fisher Bench



Targets, trig diagrams and report cards often unitary, focused...

E.G. shame factors in grey useful, but may also indicate negentropic opportunity.

In Jaynes program Frequentist orthodoxy re-enters mainly at end –receptor.

For example in our boreal soil-to-sea working group, CDOM in RASM.

Relationship to Denning Diagram

DOE Often Tries to Quantify...

Research attention vs. import

Resembles Shannon-Brillouin Scale

Just a sign flip

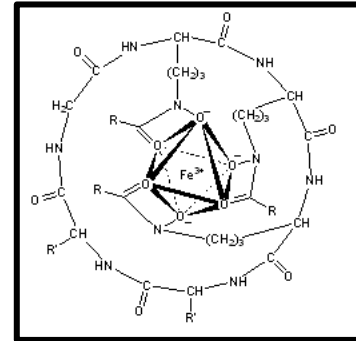
(Negentropy is tricky)

Allows Introduction of Opportunity Peak

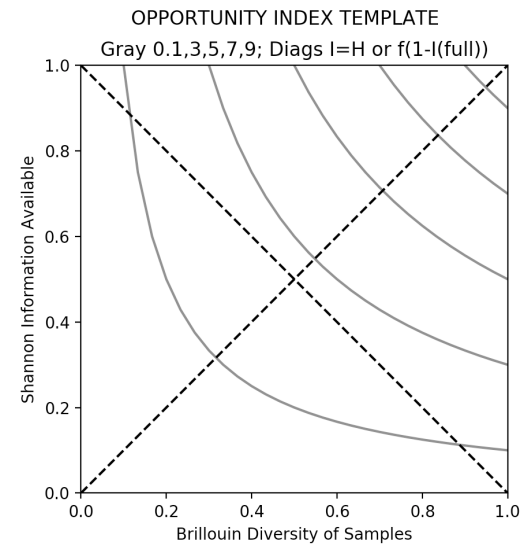
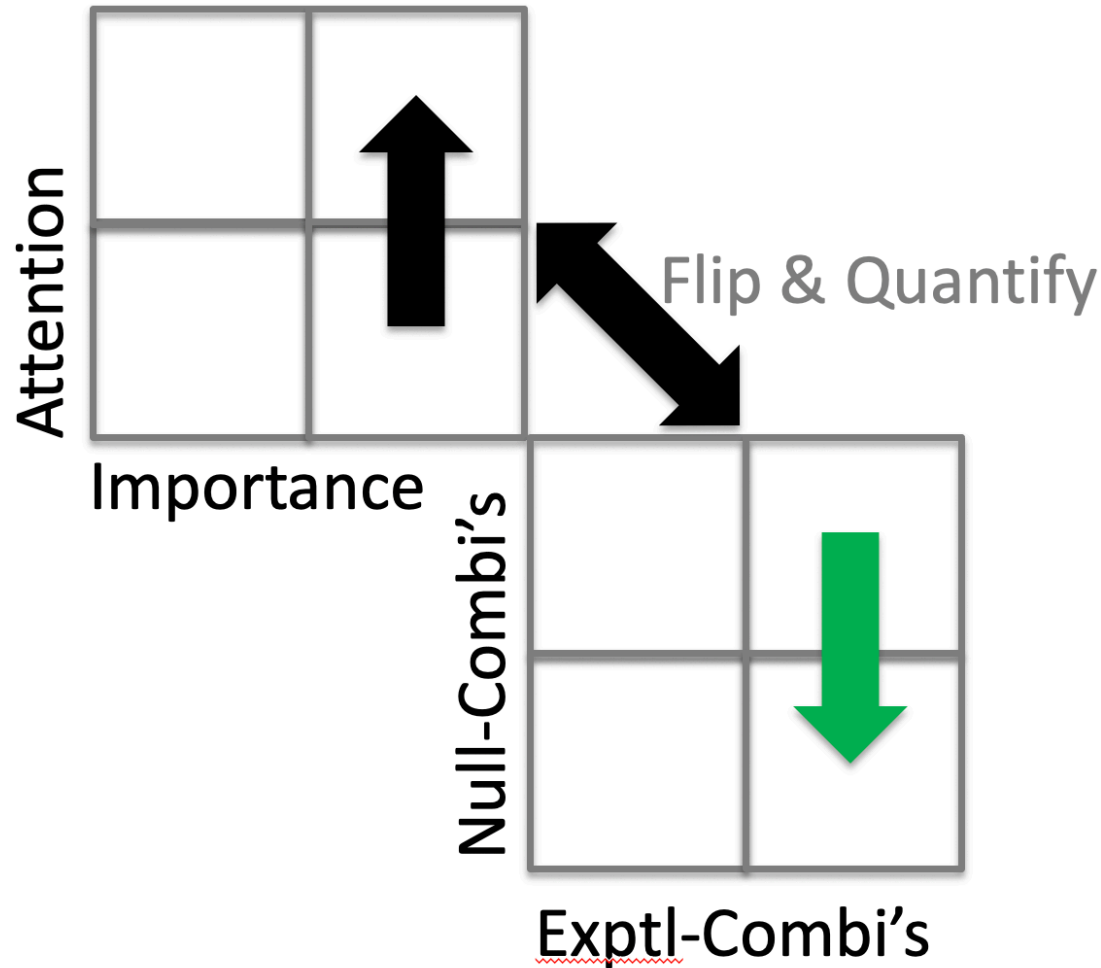
Multiply I_{avail} by $I_{diversity}$

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$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Denning and Infer-Matic Opportunity



Documentation: Recent Titles, Sources

Elliott, S. and the OBER Soil to Sea Working Group 2021. Arctic aquatic carbon cycle demonstrates Jaynesian environmental chemical filtering. In preparation for *Elementa*.

Elliott, S., Mace, J., Henson, B., and Kober, E. 2021. Jaynesian analysis of classic nitramine chemistry with entropic EOS. In preparation for *Entropy*.

Elliott, S., Holland, T., and Messerly, R. 2020. Revisiting classic radiation chemistry: Tritium drives industrial exchange of light gases. *LANL Technical Report* LA-UR-20-29029.

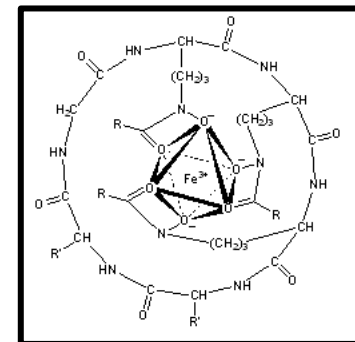
Elliott, S. with 20 others 2020. Chemistry of high energy pulses to the Earth surface environment: Overview for next generation simulation. *LANL Technical Report* LA-UR-20-26027.

Jayasinghe, A., **S. Elliott** and 6 others 2020. Modeling functional organic chemistry in Arctic rivers. *Atmosphere*, 11(10), 10.3390/atmos11101090.

Elliott, S. and 7 others 2019. Biogeochemical equation of state for the sea-air interface. *Atmosphere*, 10(5), 10.3390/atmos10050230.

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$



Jaynes Enviro-Chem: Future Community

Complements Numerous, Diverse

Prior-Systems Models

Manageable Ranked Processes

Bypass Cromwell's curse

Packaging for DOE Teams

Corrosion and aging –DRACO

Integrate Soil to Sea –E3SM Components

Integrate new ESM EOS -Surfactants

Multiphysics Pulses –E.G. SAIC family

Nitramines and HE spectrum –Safety

$$P(H | E) = \frac{P(E | H) \cdot P(H)}{P(E)}$$

$$H' = - \sum_{i=1}^S p_i \ln p_i$$

